SACADA Database Code: 508

Topology: 4^6T46

# of independent nodes (IN): 6
Transitivity: [6(12)(11)5]
Space Group: Cc
Pearson: mS24
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^6T46 (SACADA #508)		3.306		1.273	337.9	337.5	60.5	SACADA[1]
G221								doi: 10.1002/cphc.201700151

Elasticity tensor (kBar)[1]

8440.5215	1415.8761	730.4668	-0.0001	-0.0000	-300.9030
1415.8761	8368.2808	968.7003	-0.0001	-0.0001	330.0092
730.4668	968.7003	7478.1478	-0.0000	-0.0001	-242.9324
-0.0001	-0.0001	-0.0000	3351.7355	-75.4120	-0.0000
-0.0000	-0.0001	-0.0001	-75.4120	3572.3624	-0.0001
-300.9030	330.0092	-242.9324	-0.0000	-0.0001	2948.5041

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].